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Diaquabis(ethylenediamine-κ^2N,N')copper(II) bis(4-aminonaphthalene-1-sulfonate) dihydrate

Ming-Tian Li, Cheng-Gang Wang,* Yu Wu and Xu-Cheng Fu

Department of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China

Correspondence e-mail:
wangcg23@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.120
Data-to-parameter ratio = 14.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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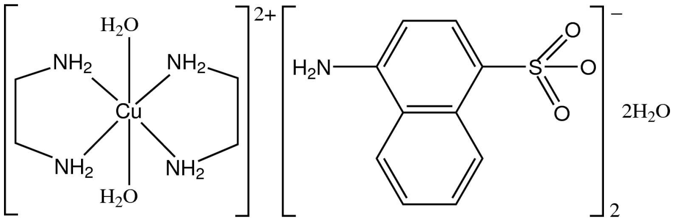
In the title compound, $[Cu(C_2H_8N_2)_2(H_2O)_2](C_{10}H_8NO_3S)_2\cdot 2H_2O$, the Cu^{II} complex cation, located on an inversion centre, has a distorted octahedral coordination geometry formed by two ethylenediamine and two water molecules. The distance of 3.4987 (11) Å between the centroids of neighbouring parallel aromatic rings of aminonaphthalenesulfonate anions suggests the existence of π–π stacking.

Comment

The sulfonate anion usually acts as a counter-ion in metal complexes (Chen *et al.*, 2002). As part of an investigation of the coordination ability of the sulfonate anion, we present here the crystal structure of the title compound, (I).



(I)

The crystal structure of (I) consists of Cu^{II} complex cations, 4-aminonaphthalene-1-sulfonate anions and solvent water molecules. The structure of (I) is shown in Fig. 1. The Cu^{II} atom, located on an inversion centre, has a distorted octahedral coordination geometry, formed by two ethylenediamine (en) and two coordinated water molecules. The Cu—N bond distances in the equatorial plane agree with those found in another $[Cu(en)_2(H_2O)_2]^{2+}$ complex (Cai, Chen *et al.*, 2001; Cai, Feng & Hu, 2001). The axial Cu—O bond distance is much longer than the Cu—N bond distances in the equatorial plane, as a result of the Jahn–Teller distortion (Table 1).

An extensive hydrogen-bonding network occurs in the crystal structure of (I) (Fig. 2 and Table 2). π–π stacking is observed between neighbouring parallel naphthalene rings, the distance between centroids being 3.4987 (11) Å for C3- and $C8^{vi}$-containing rings [symmetry code: (vi) $1 - x, -y, -z$].

Experimental

Ethylenediamine (0.12 g, 2 mmol) was added to an aqueous solution (20 ml) of $CuCl_2\cdot 2H_2O$ (0.17 g, 1 mmol). After the mixture had been stirred for 2 h at room temperature, the solution was mixed with an ethanol solution (10 ml) of sodium 4-aminonaphthalene-1-sulfonate tetrahydrate (0.32 g, 1 mmol). Blue single crystals of (I) were obtained after one week.

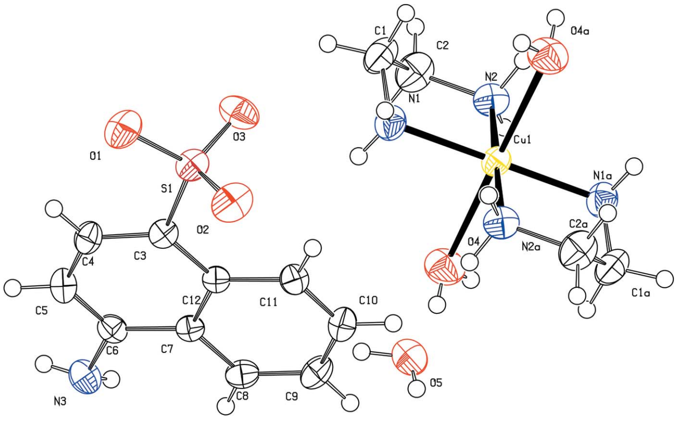


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids [symmetry code: (*a*) $-x$, $-y$, $1 - z$].

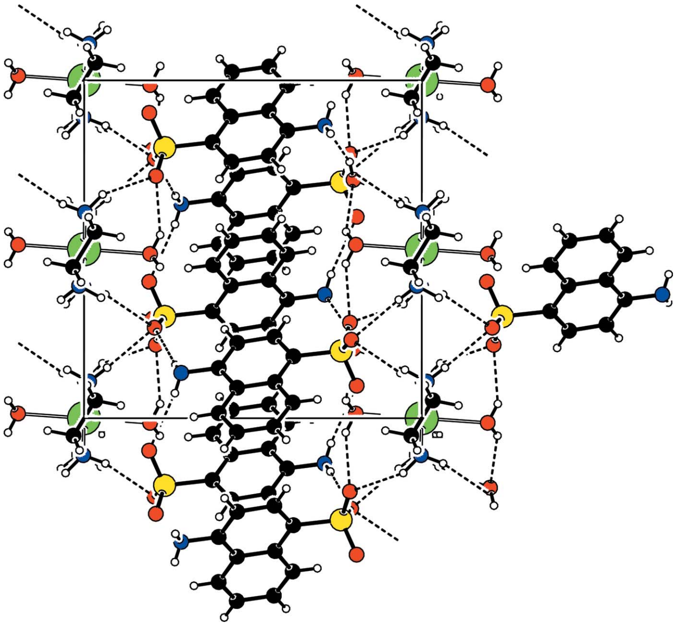


Figure 2
The packing, showing π–π stacking and the hydrogen bonding (dashed lines).

Crystal data

$[Cu(C_2H_8N_2)_2(H_2O)_2]$-$(C_{10}H_8NO_3S)_2 \cdot 2H_2O$
$M_r = 700.28$
Monoclinic, $P2_1/c$
$a = 12.4376$ (9) Å
$b = 9.5950$ (7) Å
$c = 12.4375$ (9) Å
$\beta = 90.03$ (1)°
$V = 1484.28$ (19) Å^3
$Z = 2$
$D_x = 1.567$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4417 reflections
$\theta = 2.3$–28.1°
$\mu = 0.94$ mm^{-1}
$T = 292$ (2) K
Block, blue
0.26 × 0.26 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
9813 measured reflections
3382 independent reflections
2836 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
$\theta_{\rm max} = 27.5°$
$h = -9 \rightarrow 16$
$k = -12 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.120$
$S = 1.08$
3382 reflections
236 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.39$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.48$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.0323 (19)	Cu1—O4	2.437 (2)
Cu1—N2	2.0119 (19)		
N2—Cu1—N1	84.30 (9)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O1	0.81 (3)	2.18 (3)	2.899 (3)	148 (3)
O4—H4*B*···O5$^{\rm i}$	0.77 (3)	2.24 (3)	2.888 (3)	142 (3)
O5—H5*A*···N3$^{\rm ii}$	0.87 (3)	2.03 (3)	2.875 (3)	162 (4)
O5—H5*B*···O1$^{\rm iii}$	0.77 (4)	2.13 (4)	2.877 (3)	165 (5)
N1—H1*A*···O1$^{\rm iv}$	0.95 (3)	2.27 (3)	3.143 (3)	152 (2)
N1—H1*B*···O2$^{\rm i}$	0.88 (2)	2.51 (3)	3.327 (3)	155 (2)
N2—H2*A*···O2	0.86 (2)	2.37 (3)	3.155 (3)	153 (2)
N2—H2*B*···O5$^{\rm v}$	0.92 (3)	2.06 (3)	2.967 (3)	173 (3)
N3—H3*A*···O3$^{\rm vi}$	0.78 (2)	2.33 (3)	3.100 (3)	170 (2)
N3—H3*B*···O2$^{\rm vii}$	0.80 (2)	2.59 (3)	3.381 (3)	169 (2)

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, y + 1, z$; (iv) $-x, -y, -z + 1$; (v) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (vi) $-x + 1, -y, -z$; (vii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.

The water H atoms and amine H atoms were located in a difference Fourier map and refined with the restraints O—H = 0.82 (5) Å and N—H = 0.86 (5) Å, and $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(carrier). H atoms on C atoms were placed in geometrically idealized positions and refined in riding mode, with C—H = 0.93 or 0.97 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C). We attempted to solve the structure with orthorhombic space groups but obtained no reasonable solution.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2005). E**61**, m1660–m1661 Li *et al.* • $[Cu(C_2H_8N_2)_2(H_2O)_2](C_{10}H_8NO_3S)_2 \cdot 2H_2O$ **m1661**